Elastic kMC Simulation of Radiation Damage

Toby Hudson, **Adrian Sutton**, *University of Oxford*
María-José Caturla, *Lawrence Livermore National Laboratory*
Sergei Dudarev, *U. K. Atomic Energy Agency*

The kinetic Monte Carlo (kMC) method has already proven an invaluable technique for simulating materials on longer timescales than molecular dynamics can attain. The simulation of accumulated high energy radiation damage to metals, a process especially relevant to both fission and fusion reactors, requires such timescales. Until now kMC simulations of this damage have treated the fast diffusing interstitials, vacancies and small dislocation loops generated by the irradiation as pure Brownian motion in either one or three dimensions. In reality however, they experience long range elastic interactions which bias the stochastic diffusion. We have incorporated elastic interactions into our kMC simulation, and hence can discuss some of the consequences this has for the overall evolution of the irradiated material.
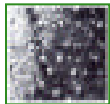
Background
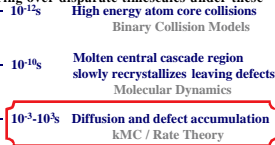
Radiation Damage in Metals

Radiation has many effects on metals including:
embrittlement **swelling** **plastic instability**

It is vitally important to understand the effects of radiation out to the high energy (14MeV), high fluence conditions expected for the structural materials in magnetic and inertial confinement fusion.
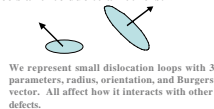
There are substantial challenges for modeling the materials processes occurring over disparate timescales under these conditions:

10^{-12}s — **High energy atom core collisions**
Binary Collision Models

10^{-10}s — **Molten central cascade region slowly recrystallizes leaving defects**
Molecular Dynamics

10^{-3}-10^{3}s — **Diffusion and defect accumulation**
*kMC / Rate Theory*

time

Elastic Interactions

Defects do not diffuse freely! Any defect feels a force due to all others:

✦ **A stress and strain is generated around each defect to better accommodate it, and minimize the overall potential energy. These fields have no characteristic length, and thus can act over long distances.**

A) We represent small dislocation loops with 3 parameters, radius, orientation, and Burgers vector. All affect how it interacts with other defects.

✦ **When the stress field of one defect overlaps with that of another, there is an extra net energy cost or gain. This is referred to as the elastic interaction energy between the two defects.**

The energy depends on A) the shape, orientation and nature of the defects, as well as B) the elastic properties of the crystal.
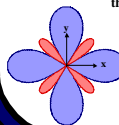
B) Elastic energy contour between two spherically symmetric point defects in an anisotropic cubic crystal (001) crystal plane
Repulsion / Attraction

If linear elasticity is assumed, analytic expressions for this energy can often be obtained for particular types of defect. We use Eshelby 1955, and Khraishi et al 2001 to study point defects and loops.
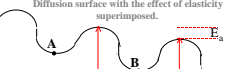
Simulations

Kinetic Monte Carlo

Diffusion surface as standard kMC would see it.
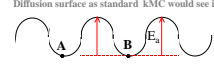
Diffusion surface with the effect of elasticity superimposed.

Benefits of kMC
- captures long timescale effects (unlike molecular dynamics)
- includes stochastic nature of diffusive motion (unlike dislocation dynamics)

Elasticity in kMC
- primarily affects the diffusion of mobile species
- a full treatment would include altering the shapes of reaction capture regions.

$$\alpha = 1 - \frac{2\exp-\dfrac{E_a}{2kT}}{\exp-\dfrac{E_a}{2kT}+\exp-\dfrac{E_a}{2kT}}$$

Elasticity is incorporated as a bias to the diffusion by allowing a certain fraction α of the uphill diffusive hops to exactly reverse their direction (now downhill). The net frequency of diffusive hops remains the same as that without elasticity.

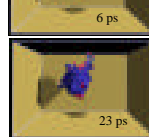α is chosen In order to satisfy the principle of microscopic reversibility.

System: Irradiation Cascade

0.06 ps

6 ps

23 ps
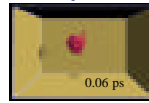
MD simulations of the initial few picoseconds of a high energy cascade cover the period in which local melting and recrystallization occurs.

We use the eventual configuration of defects thus generated as our input for kMC simulations.

In this study, we have used 7 different cascades in iron at 500K generated by a primary knock on atom with an energy of 10 keV.
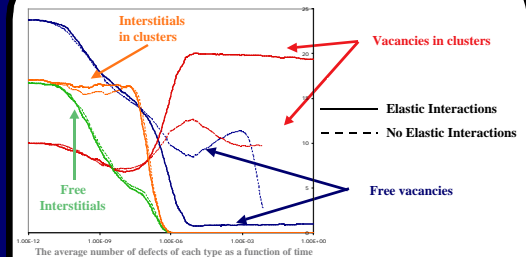[Stoller and Calder 2000]

Typical energetics and attempt frequencies for defect motion and reaction were used in both the Elastic and non-Elastic KMC.
[Soneda and Diaz de la Rubia 2001]

Each configuration is also run 10 times with different random number seeds in order to further increase the sample size.

Discussion

Initial Results

Interstitials in clusters

Vacancies in clusters

Free Interstitials

Elastic Interactions

No Elastic Interactions

Free vacancies

The average number of defects of each type as a function of time

Late stages of cascade evolution show vacancies substantially more clustered when elastic interactions are included.

This means they take much longer to escape the volume surrounding the cascade.

Conclusions

Linear elastic interactions have been included in a kMC framework.

The importance of these interactions for modeling radiation damage was demonstrated through the example of the diffusive evolution of a single 10 keV cascade at 500K.

Substantial enhancements in the clustering behavior of vacancies were observed when elastic interactions were included.

J. D. Eshelby, The elastic interaction of point defects, *Acta. Met.* **3** (1955) 487-490.
T. A. Khraishi, H. M. Zbib, T. Diaz de la Rubia, M. Victoria, Modelling of irradiation-induced hardening in metals using dislocation dynamics, *Phil. Mag. Lett.* **81** (2001) 583-593
R. E. Stoller, A. F. Calder, Statistical analysis of a library of molecular dynamics cascade simulations in iron at 100 K, *J. Nucl. Mater.* **283** (2000) 746-752
N. Soneda, T. Diaz de la Rubia, Migration kinetics of the self-interstitial atom and its clusters in bcc Fe. *Phil. Mag.* A **81** (2001) 331-343.